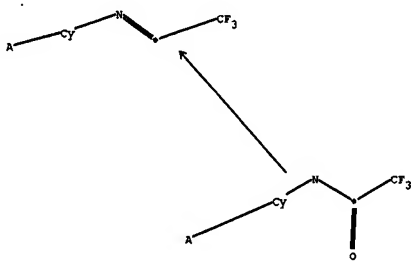
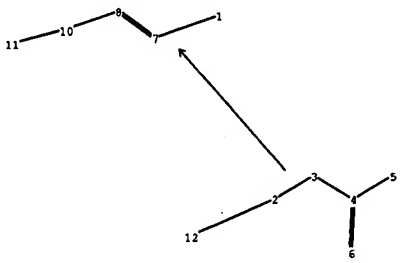
C:\Program Files\Stnexp\Queries\573.str




L6




chain nodes :
1 2 3 4 5 6 7 8 10 11 12
chain bonds :
1-7 2-3 2-12 3-4 4-5 4-6 7-8 8-10 10-11
exact/norm bonds :
2-3 2-12 3-4 4-6 7-8 8-10 10-11
exact bonds :
1-7 4-5

Match level :
1:CLASS 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 10:Atom 11:CLASS 12:CLASS
Generic attributes :
2:
Saturation : Unsaturated
10:
Saturation : Unsaturated

fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 2

CAS ONLINE PRINTOUT

=> d his

(FILE 'HOME' ENTERED AT 09:25:19 ON 23 APR 2007)

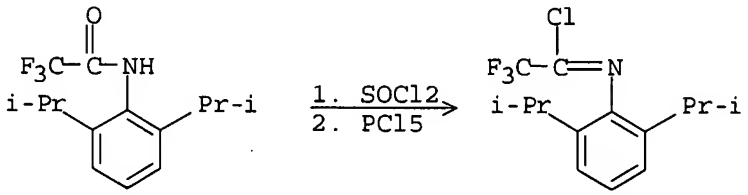
FILE 'REGISTRY' ENTERED AT 09:25:25 ON 23 APR 2007
E PHOSPHOROUS OXYCHLORIDE/CN
L1 1 S E4
E PHOSPHORIC TRICHLORIDE/CN
L2 1 S E3
E DIPHENYL CHLOROPHOSPHATE/CN
L3 1 S E3

FILE 'CASREACT' ENTERED AT 09:27:46 ON 23 APR 2007
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 4 S L6 FUL

=> d crdref 1-4

L8 ANSWER 1 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 10

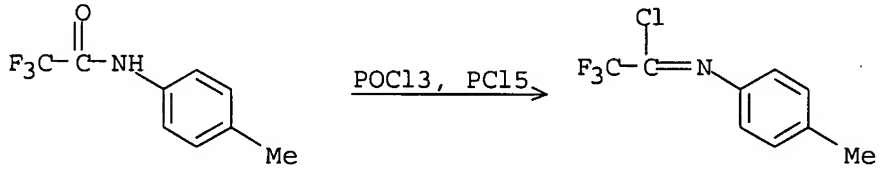



(step 1) 63%

REF: Canadian Journal of Chemistry, 78(5), 583-589; 2000

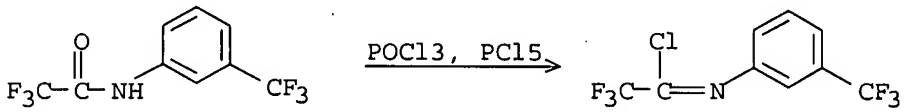
L8 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3




REF: Khimiko-Farmatsevticheskii Zhurnal, 30(11), 26-28; 1996

RX(3) OF 3

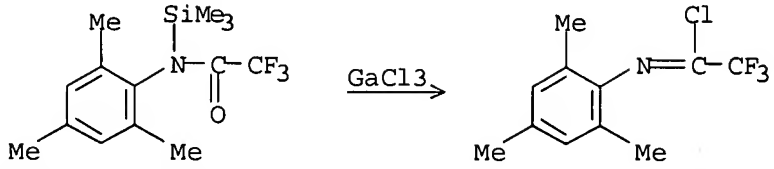



REF: Khimiko-Farmatsevticheskii Zhurnal, 30(11), 26-28; 1996

CAS ONLINE PRINTOUT

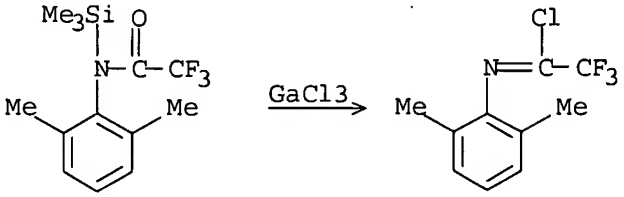
L8 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 9




REF: Monatshefte fuer Chemie, 111(5), 1087-96; 1980

RX(8) OF 9



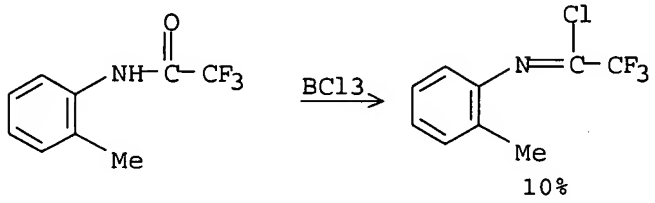

REF: Monatshefte fuer Chemie, 111(5), 1087-96; 1980

L8 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 88


REF: Monatshefte fuer Chemie, 110(1), 63-88; 1979

RX(29) OF 88

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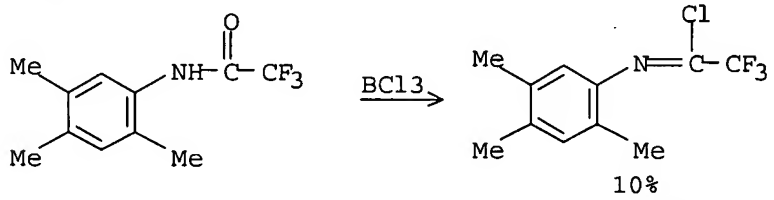
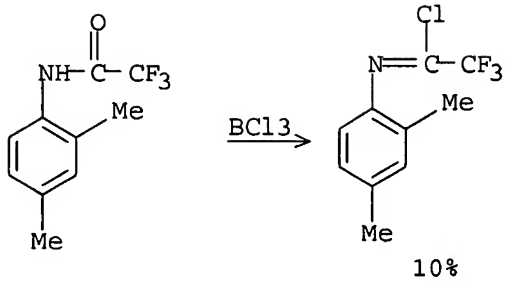
RX(30) OF 88




REF: Monatshefte fuer Chemie, 110(1), 63-88; 1979

CAS ONLINE PRINTOUT

RX(48) OF 88

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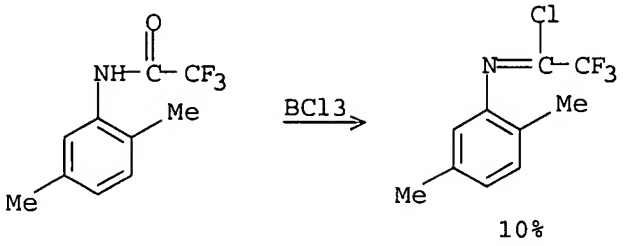
REF: Monatshefte fuer Chemie, 110(1), 63-88; 1979

RX(49) OF 88

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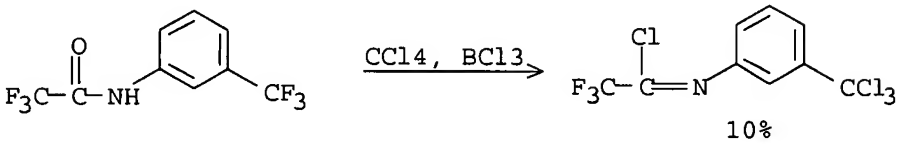
RX(50) OF 88

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REF: Monatshefte fuer Chemie, 110(1), 63-88; 1979

=>

CAS ONLINE PRINTOUT

```
=> d his

     (FILE 'HOME' ENTERED AT 09:25:19 ON 23 APR 2007)

     FILE 'REGISTRY' ENTERED AT 09:25:25 ON 23 APR 2007
                E PHOSPHOROUS OXYCHLORIDE/CN
L1            1 S E4
                E PHOSPHORIC TRICHLORIDE/CN
L2            1 S E3
                E DIPHENYL CHLOROPHOSPHATE/CN
L3            1 S E3

     FILE 'CASREACT' ENTERED AT 09:27:46 ON 23 APR 2007
L4              STRUCTURE UPLOADED
L5            0 S L4
L6              STRUCTURE UPLOADED
L7            0 S L6
L8            4 S L6 FUL

     FILE 'REGISTRY' ENTERED AT 09:31:34 ON 23 APR 2007
L9           22 S TERTIARY AMINE

     FILE 'CASREACT' ENTERED AT 09:34:16 ON 23 APR 2007
L10        1579 S TERTIARY AMINE

=> s l10 and l8
L11           0 L10 AND L8

=>
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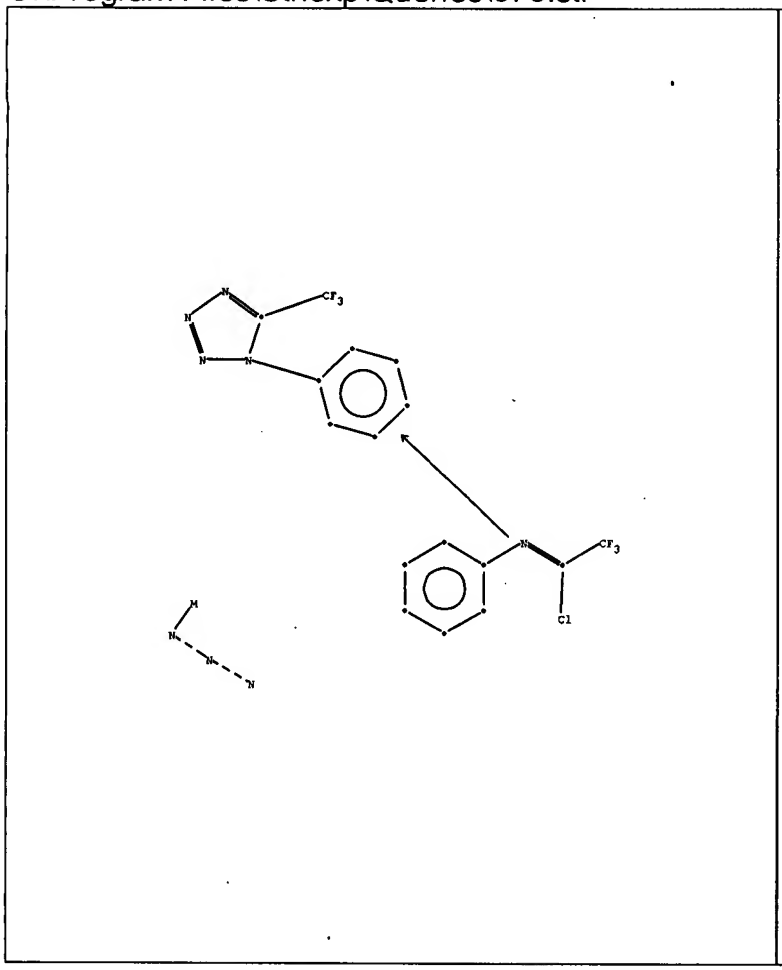
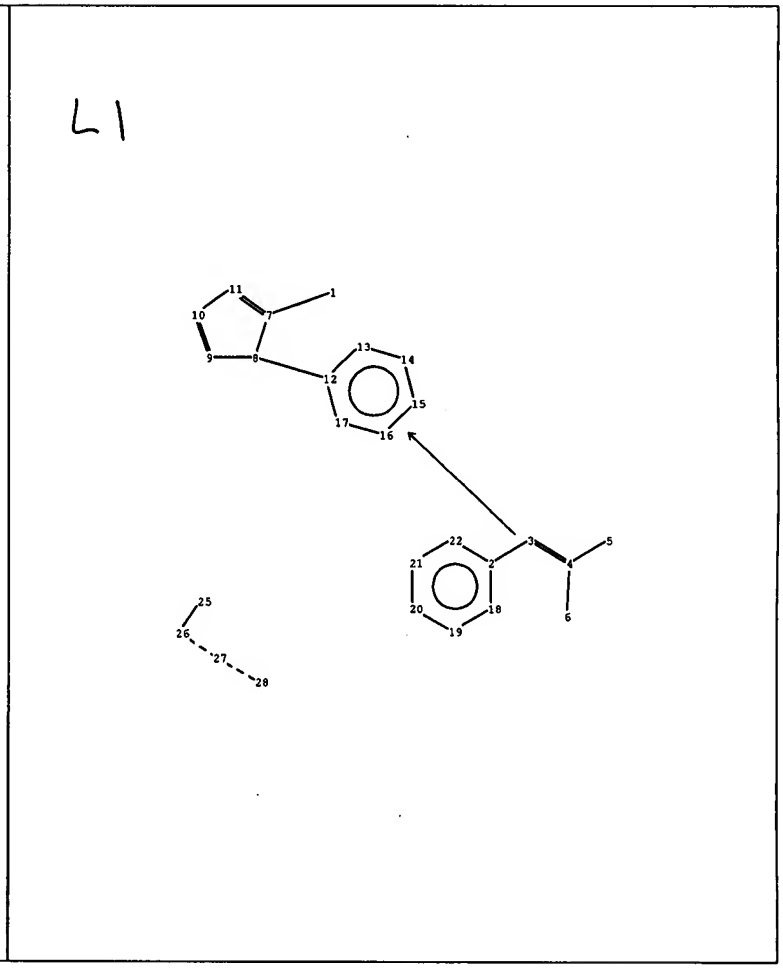
C:\Program Files\Stnexp\Queries\573.str






chain nodes :
1 3 4 5 6 25 26 27 28
ring nodes :
2 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
1-7 2-3 3-4 4-5 4-6 8-12 25-26 26-27 27-28
ring bonds :
2-18 2-22 7-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17 18-19 19-20 20-21 21-22
exact/norm bonds :
2-3 3-4 7-8 7-11 8-9 8-12 9-10 10-11 26-27 27-28
exact bonds :
1-7 4-5 4-6 25-26
normalized bonds :
2-18 2-22 12-13 12-17 13-14 14-15 15-16 16-17 18-19 19-20 20-21 21-22

Match level :
1:CLASS 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:

containing 2
containing 25

CAS ONLINE PRINTOUT

=> d his

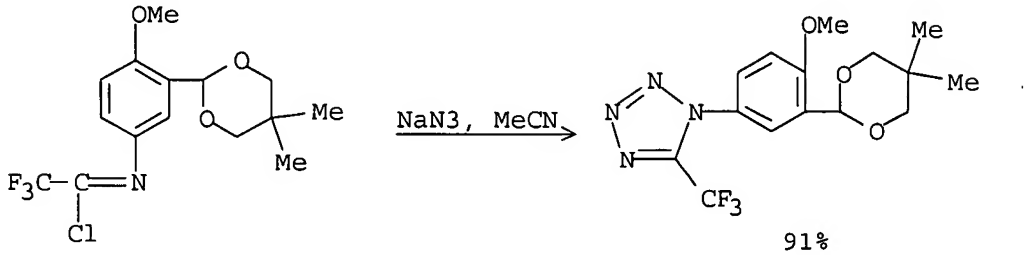
(FILE 'HOME' ENTERED AT 09:48:18 ON 23 APR 2007)

FILE 'CASREACT' ENTERED AT 09:48:40 ON 23 APR 2007
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 2 S L1 FUL

=> d crdref 1-2

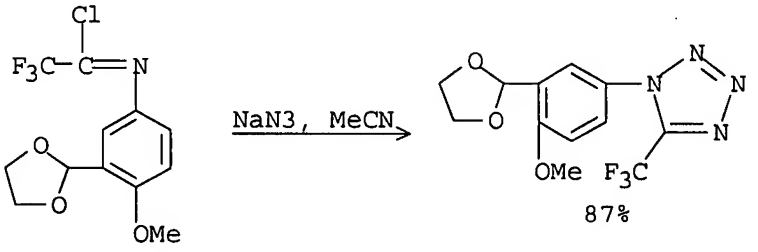
L3 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(14) OF 81



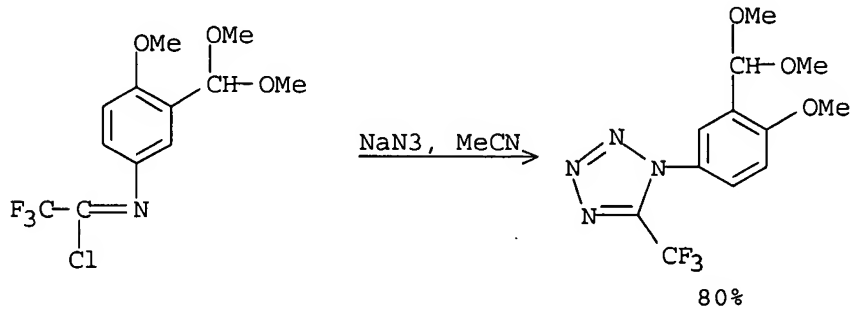

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1850810, 25 Oct 2006
CON: room temperature

RX(15) OF 81




REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: room temperature

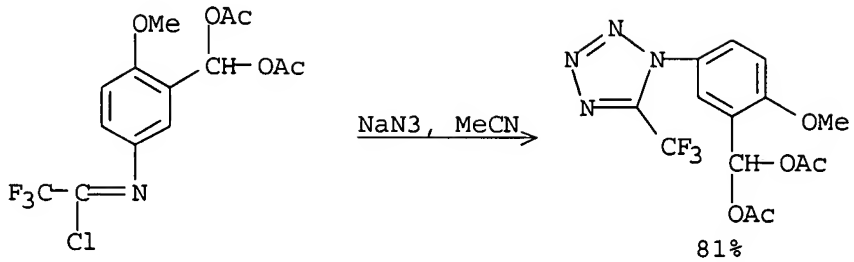
RX(16) OF 81




REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: room temperature

CAS ONLINE PRINTOUT

RX(17) OF 81

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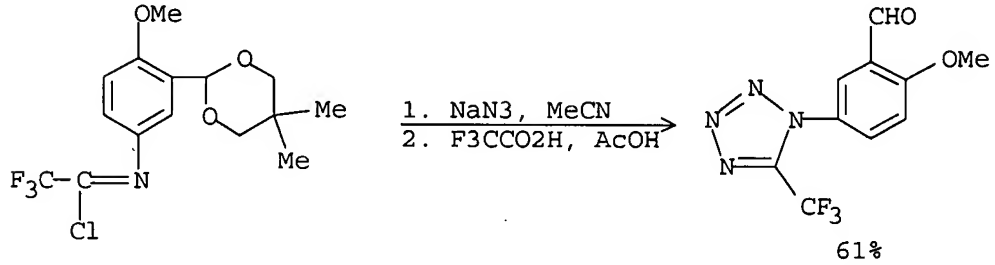
REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: room temperature

RX(38) OF 81 - 2 STEPS

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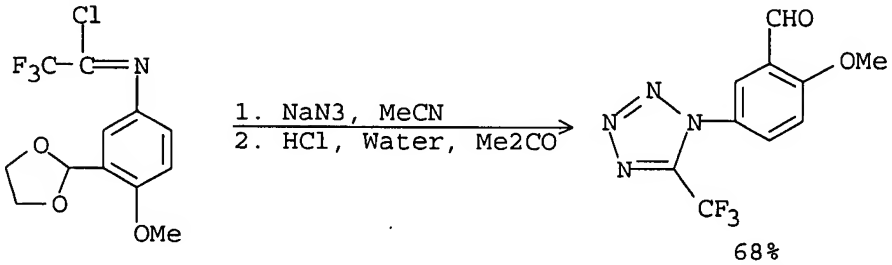
REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: STEP(1) room temperature
STEP(2) reflux

RX(39) OF 81 - 2 STEPS

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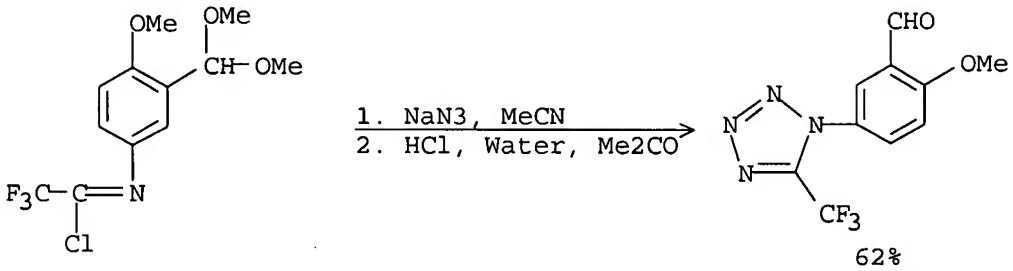
REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: STEP(1) room temperature
STEP(2) room temperature

CAS ONLINE PRINTOUT

RX(40) OF 81 - 2 STEPS

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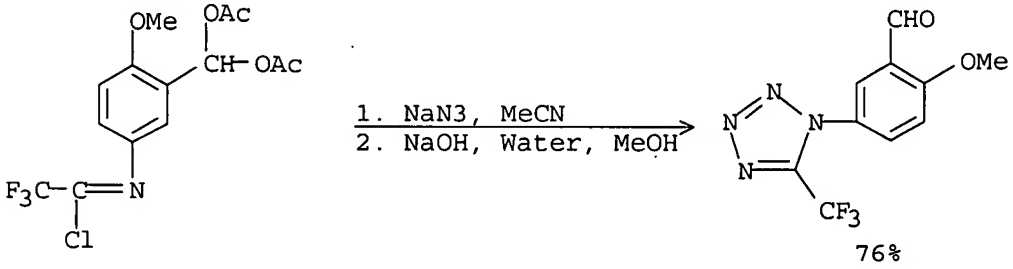
REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: STEP(1) room temperature
STEP(2) room temperature

RX(41) OF 81 - 2 STEPS

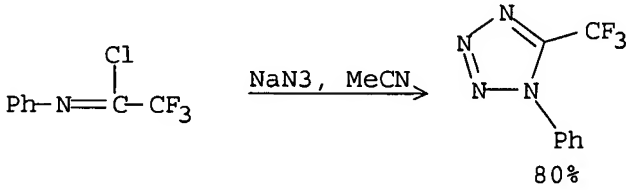



76%

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11pp.; 2006
CON: STEP(1) room temperature
STEP(2) reflux

L3 ANSWER 2 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

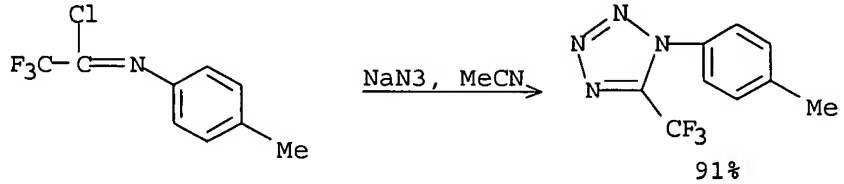
RX(1) OF 12




80%

REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

RX(2) OF 12

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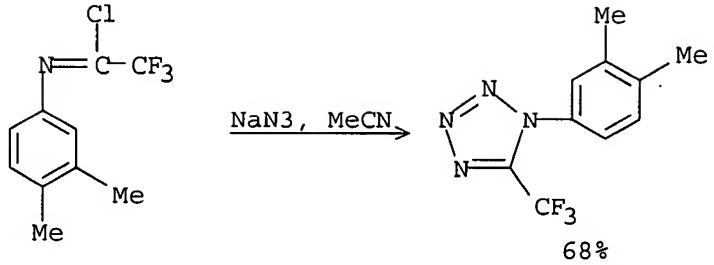
REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

CAS ONLINE PRINTOUT

RX(3) OF 12

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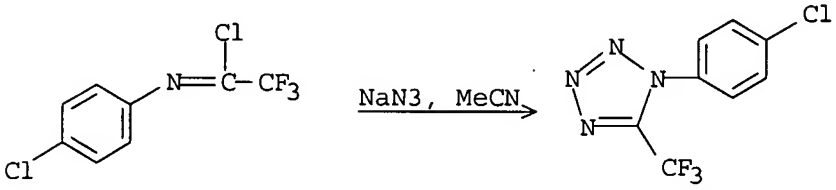
REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

RX(4) OF 12

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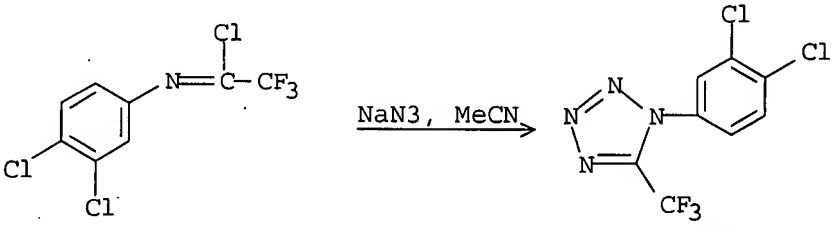
RX(5) OF 12

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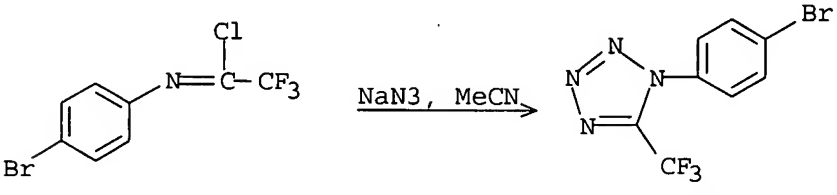
RX(6) OF 12

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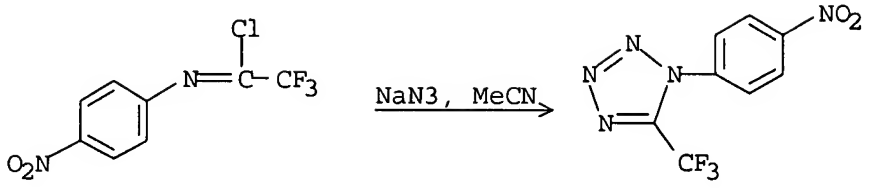
REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

CAS ONLINE PRINTOUT

RX(7) OF 12

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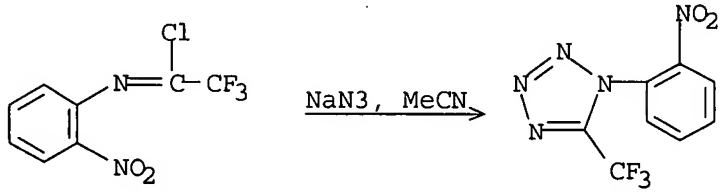
REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

RX(8) OF 12

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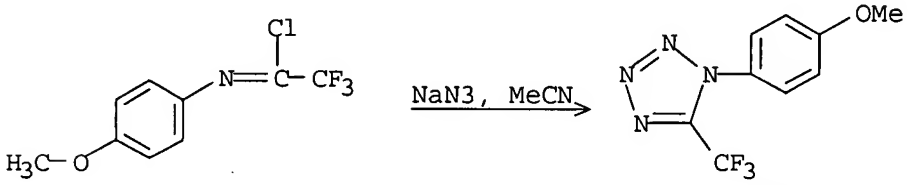
REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

RX(9) OF 12

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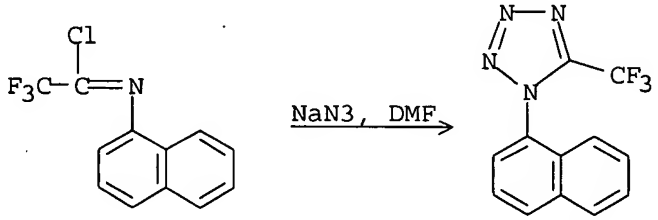
RX(12) OF 12

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REF: Journal of Fluorine Chemistry, 99(1), 83-85; 1999

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